

ATM Accessory

- Users Manual
Version 003



This Manual was written by

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1 Introduction

1.1 General Description

This manual describes the ATM (Automatic Tuning and Matching) Accessory for probe-heads with selective, tunable, broad-band and switched channels. The ATM Accessory consists of hardware, which is part of the probe or an option, and some commands in the TopSpin software.

The ATM Accessory allows to optimize the tuning and matching automatically for each sample.

1.2 ATM Features

- Automatic matching and tuning of all routed nuclei (nucleus must be observable)
- Optimal performance (S/N) in automation, e.g. when using a sample changer
- Easy manual matching and tuning via remote software control
- Automatic nucleus change on broad-band and switched probes
- Easy set up for new nuclei on broad-band and switched probes
- Elegant installation of probe heads equipped with ATM Accessory into the magnet without the need for mechanical adjustments

1.3 Scope of this Manual

This manual describes the current state of hardware and software at the release date.

This is the included hardware and software:

Unit	Version
Spectrometer	AVANCE series
ATM for RT probes	all
ATM for Cryo Probes	all
HPPR/1	all except CRP HPPR
HPPR/2	all
Internal HPPR	all
ATMA Server	3.92
TOPSPIN	2.1 pl5, most ATMA features since 1.3

Table 1.1: Hardware and Software Described in this Manual

1.4 The Two Different ATM Types

There are different ATM Accessories for RT probes or CryoProbes, but the control with TOPSPIN is exactly the same

Difference	RT probe ATM Accessory	CRP ATM Accessory
Actuator	The actuator unit is permanently mounted on the probe-head.	The actuator unit can be detached from the probe.
Upgrade	Upgrading the probe head with the ATM Accessory is not possible.	The ATM Accessory can be added on newer cryo probes, even when the probe is cold.
PICS	The ATM Accessory is connected and controlled by the probe head PICS.	The ATM Accessory has its own, probe head independent, PICS.
Tuning and matching adjust	Only the actuator will trim the tuning and matching.	The user can adjust the nucleus manually by installing the manual tuning and matching adapter.
Freezing	The actuator unit cannot freeze.	The ATM Accessory has an integrated bottom heater to prevent from icing on the mechanical connection.

Table 1.2: Differences Between RT and CRP ATM Accessory

2 Safety

2.1 Warnings and Notes in this Manual

There are different types of information notices used in this manual. These notices highlight important information or warn the user of a potentially dangerous situation. The following notices will have the same level of importance throughout this manual.



CAUTION

Type and source of danger

What might happen?

- „ Counter measure 1
- „ Counter measure 2
- „ ...

Indicates a hazardous situation which, if not avoided, may result in minor or moderate injury or major material damage.

NOTICE

Type and source of danger

What might happen?

- „ Counter measure 1
- „ Counter measure 2
- „ ...

Hazard, which could result in material damage.

i Information

Hints for convenient working and optimal performance of the system.

2.2 Disclaimer

- The unit should only be used for its intended purpose as described in this manual.
- Use of the unit for any purpose other than that for which it is intended is done so at the users own risk and invalidates any and all manufacturers warranties.
- Service or maintenance work on the unit must be carried out by qualified personnel.
- Only those persons trained in the operation of the ATM Accessory should operate it.
- Read this manual before operating the unit. Pay particular attention to any safety related information.

NOTICE

Disclaimer

BRUKER BIOSPIN is not responsible or liable for any injury or damage that occurs as a consequence of non-approved manipulations on the ATM Accessory.

„ Read the manual carefully before working with the ATM Accessory.

2.3 Site Considerations

The ATM Accessory should be setup in a standard laboratory environment. Maximum room temperature should not exceed the range from 17-25°C. For more information refer to the Avance spectrometer manual on site planning¹ available from BRUKER BIOSPIN.

1. See Appendix: A.5 References

3 Installation

3.1 Installations Notes



CAUTION

Magnetic attraction

In the case of a strong magnet it is possible, that the probe may be attracted.

- „ Be careful when moving the RT probe with ATM Accessory or CRP ATM Accessory near the magnet.
- „ Further information about probes can be found in Probes User Manual (BASH).

NOTICE

High torque damage probe

High torque on the mounting screws does not improve measurements but may damage the probe or ATM Accessory.

- „ Tighten the mounting screws alternately without using excessive torque and by using the special handle.

3.2 Mounting RT probe

Inserting a RT probe with attached ATM Accessory is as easy as a probe without one. The probe will be fixed to the shim system with two screws located inside the ATM Accessory. The position of these screws is the same as for probes without ATMA.

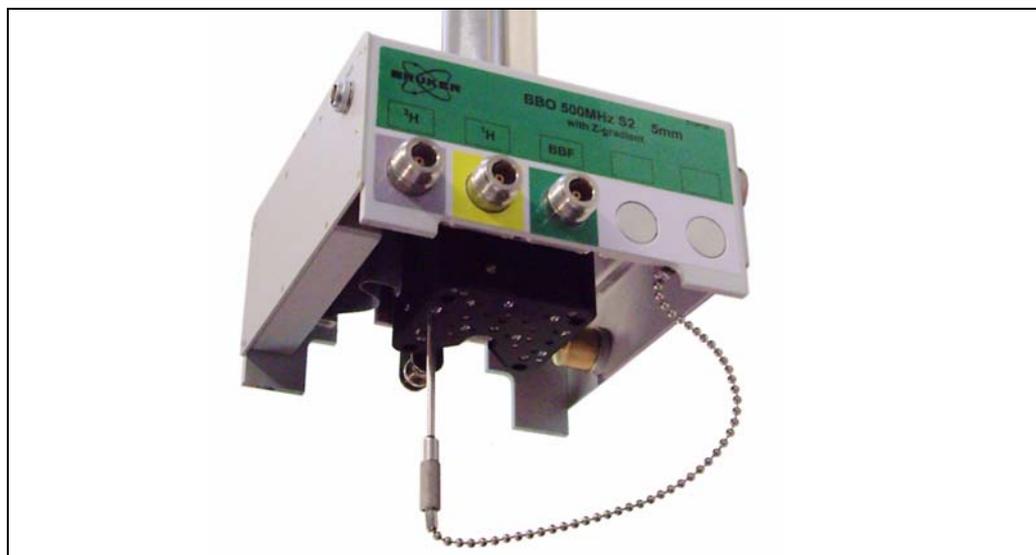


Figure 3.1: RT Probe with ATM Mounting Screws

i The mounting screws in the actuator unit are hard to find if the probe is inserted into the magnet. See the picture below and memorize the positions of the screws before mounting the probe.

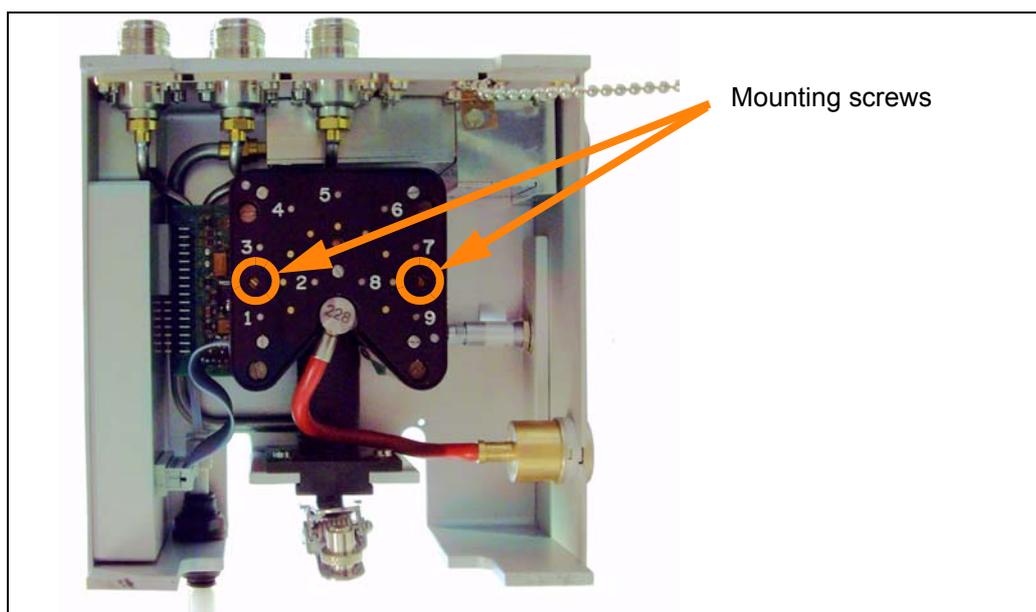


Figure 3.2: RT Probe with ATM Bottom View

3.3 Mounting CRP ATM Accessory

NOTICE

Cold CRP can warm up

When upgrading a cold probe with a ATM Accessory, the bottom heater must be switched off.

- „ Enter the service mode in CryoTool or CryoPanel and switch off the *Temp. Ctl 3 (Bottom-H)*.
- „ After this, you can detach the bottom heater cable from the mechanical tuning & matching adapter.
- „ When the ATM Accessory is mounted and bottom heater cable is connected, do not forget to switch on the *Temp. Ctl 3 (Bottom-H)* in CryoTool or CryoPanel.

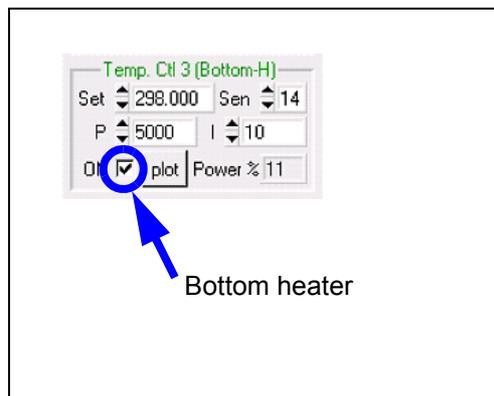


Figure 3.3: CryoTool Bottom Heater

1. Install the cryo probe into the magnet. Plug in the VT-air tube and connect the CABLE BVT-CRP (P/N Z14278).
2. While mounting the ATM actuator unit make sure that the alignment bolts are positioned correctly with the probe. Some force is required to push the ATM actuator unit to the bottom plate of the CryoProbe (to compensate the force of the springs). For this see the picture "[Cryo Probe ATM Mounting](#)" on page 14

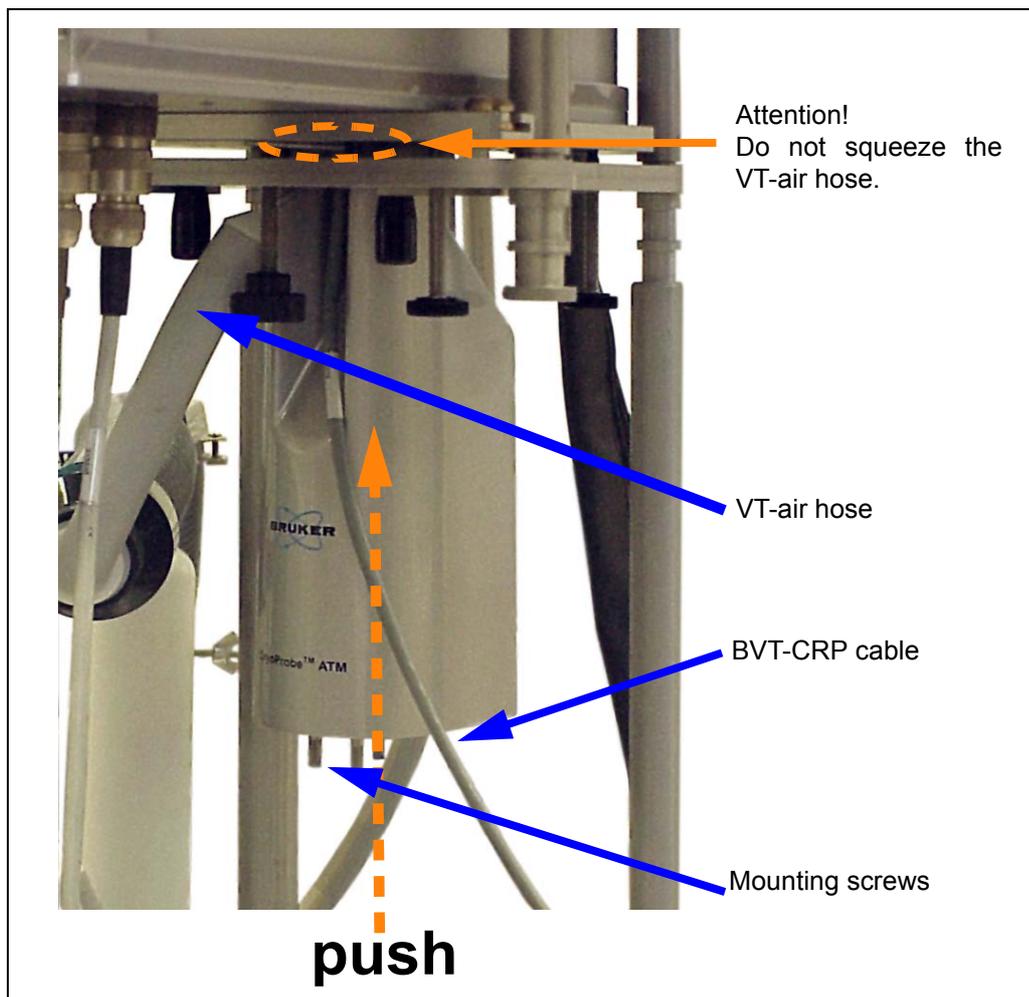


Figure 3.4: Cryo Probe ATM Mounting

3. Tighten the three screws at the bottom of the ATM actuator unit by hand.
4. Make sure not to have squeezed the VT-air hose: Check at the BVT-Unit that the air flow is still present.

3.4 Connecting the ATM Accessory

To operate the ATM Accessory a connection from the probe to the HPPR is required. Depending on the HPPR, different cables are needed

HPPR	PICS cable number	PICS cable label
HPPR/1	Z2927	HPPR/PIC SYSTEM
HPPR/2	Z14361	HPPR/2<->ATMA/PICS
Internal HPPR	Z100240	HPPR/2 - ATMA/PICS

Table 3.1: PICS Cables

For the CRP ATM actuator unit an additional cable is needed to connect the cryo cooler.

Cooler	Bottom heater cable number	Bottom heater cable label
CU/1 to CU/3	Z14374	BOTTOM ADAPTER
CU/4	Z106881	BOTTOM ADAPTER

Table 3.2: Bottom heater cables

3.4.1 HPPR connector

NOTICE

HPPR reset

Connecting while the HPPR is running, the HPPR may reset (lamps will black out).

- „ If this happens, the HPPR must be initialized by typing the command `ii` in TOPSPIN.
- „ For further details consult the TOPSPIN Software Manual.

Different HPPR have different connectors for the PICS cable. See the different HPPR with their ATMA / PICS sockets on the subsequent pages.

NOTICE

Similar sockets

Do not connect the PICS cable to the wrong socket on HPPR/2 or console.

- „ Read the labels on the HPPR/2 or console sockets carefully.

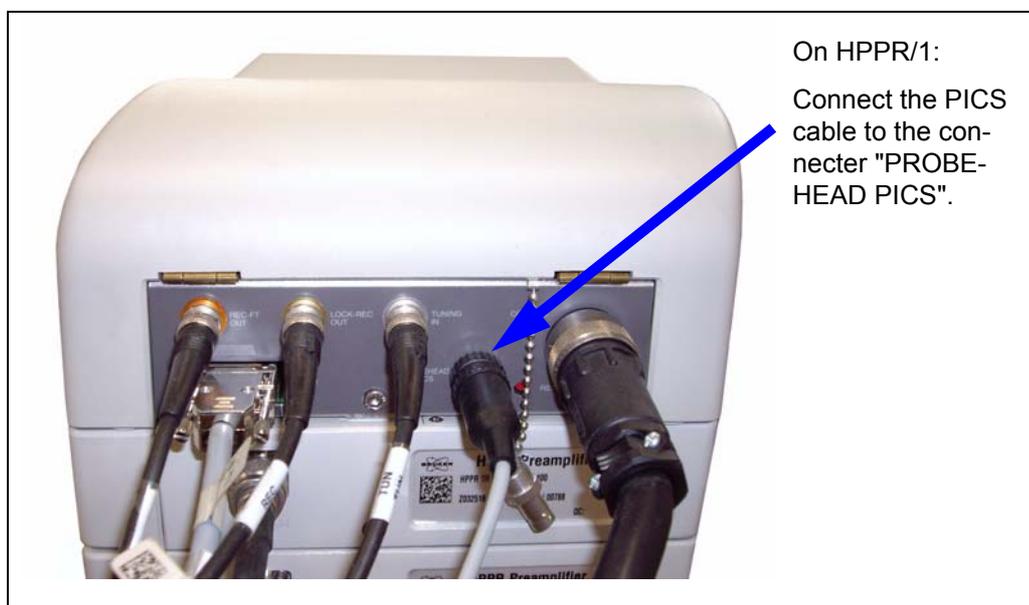
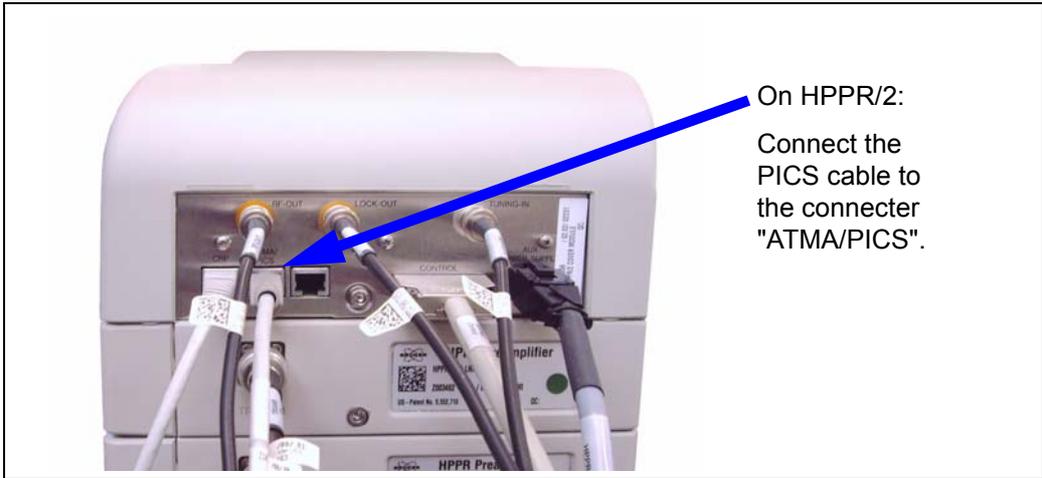
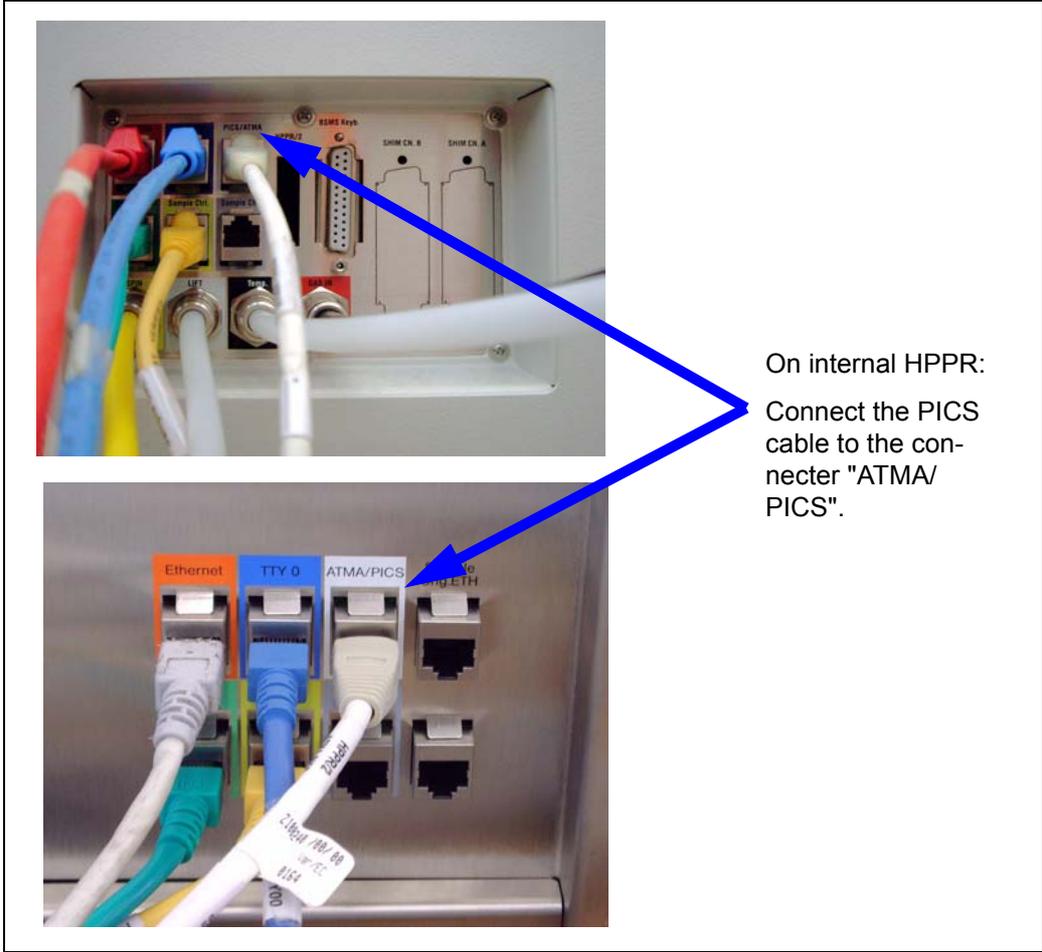


Figure 3.5: External HPPR/1



On HPPR/2:
Connect the
PICS cable to
the connector
"ATMA/PICS".

Figure 3.6: External HPPR/2



On internal HPPR:
Connect the PICS
cable to the con-
nector "ATMA/
PICS".

Figure 3.7: Internal HPPR

3.4.2 ATM / Probe Connector

Connect the PICS cable on the connector on the side of the RT probe.

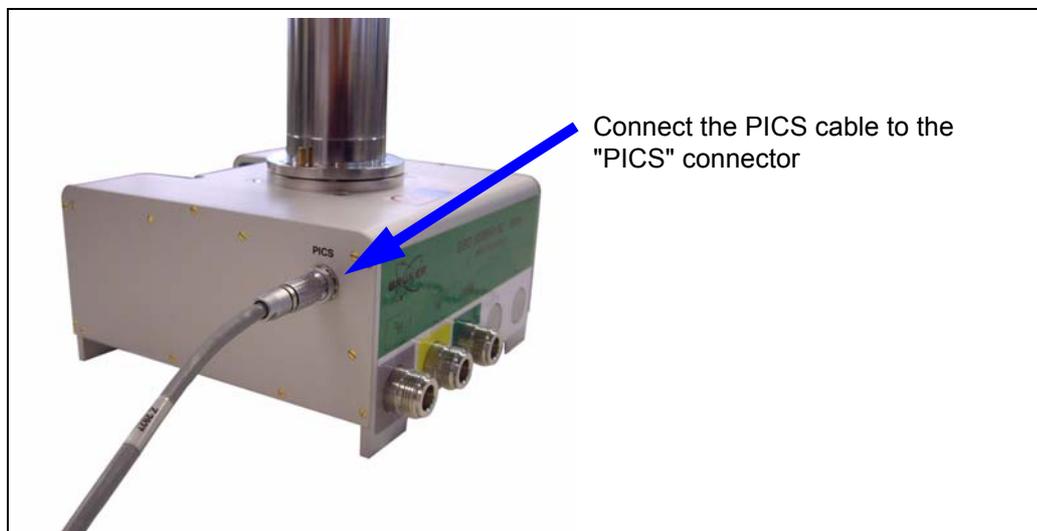


Figure 3.8: ATM PICS Connector on an RT probe

The CRP ATM actuator unit needs two cables.

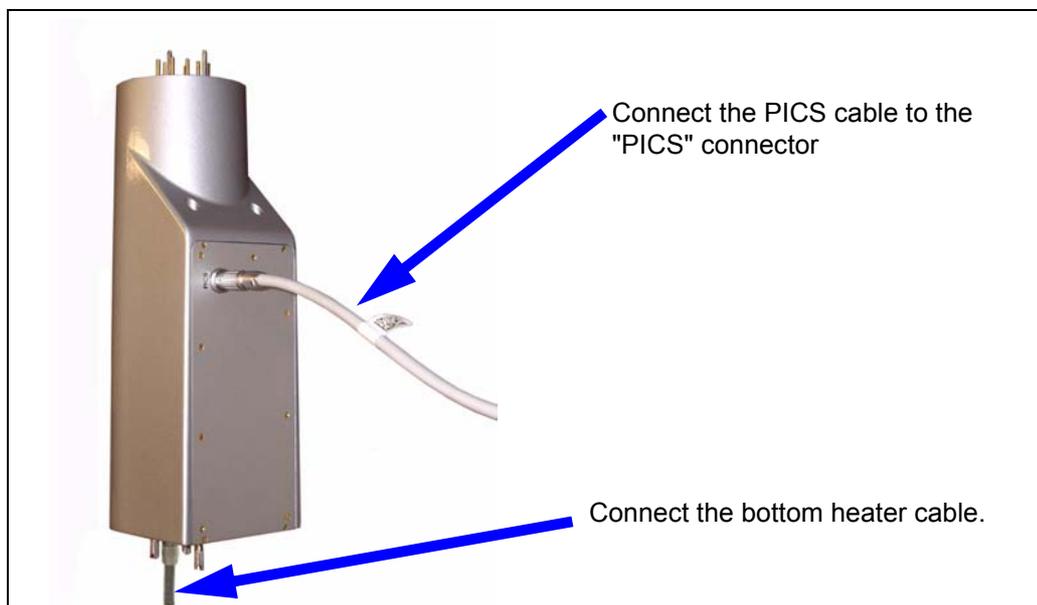


Figure 3.9: Connector on a CRP ATM actuator unit

i In TOPSPIN type **edhead** before using ATM.

4 Using ATMA

4.1 TOPSPIN commands *atma* and *atmm*

The two commands *atma* and *atmm*, integrated in TOPSPIN, are described below. Both commands relay on the *edsp* setting of the current data set.

- The command *atma* (*automatic tuning matching automatically*) is the way to get the optimal performance. It will automatically tune and match your probe, without any intervention.
- The command *atmm* (*automatic tuning matching manually*) is mainly used for verifying the current, or calibrating a new nuclei position on broad-band probes. It allows the positions of the tuning and matching rods of the probe to be operated directly via the workstation. A separate window will be opened showing various controls.

4.1.1 Remarks for *atma* and *atmm*

- Both commands, *atma* and *atmm*, will separately start the wobble procedure.
- The wobble width (*wbsw*) and the number of wobble steps (*wbst*) will be automatically defined dependent on the nucleus. After finishing of *atma* or *atmm*, the old state of *wbsw* and *wbst* will be restored. For *atmm*, user defined values can be used with the option *manWbsw*
- A special wobble procedure is started when either *atma* or *atmm* is active. It has a non equispaced frequency range and uses mostly an extended wobble sweep width. So the wobble curve may look unfamiliar.
- *atma* will stop spinning the sample to obtain optimal results. After *atma* has finished, the old state will be restored.
- Both commands will store positions for tuning and matching. The command *atma* is doing this automatically while *atmm* will ask if the values should be stored. Depending on the probe head positions for nuclei and solvents will be stored.

4.1.2 *atma* process

The command *atma* will automatically tune and match your probe, without any intervention

atma will do the following operations:

1. Check if one of the actuators is on the end stop and has to be moved away.
2. Initializing the actuators if needed (see [“Actuator Initialisation” on page 6-5-30.](#)).
3. Read the probe information from the PIC system and get information of the routed channel in TOPSPIN (e.g. *edsp*)

4. Turn off the sample rotation and set the optimal wobble width (**wbsw**) and the number of wobble steps (**wbst**) for the given channel
5. Set the broad-band or switched channels, to the configured nucleus.
6. Start a special wobble process to get the best resolution. The wobble curve may look unfamiliar
7. Optimize the tuning and matching in several optimization cycles
8. Stop the wobble process
9. Restart the process at step 4, if another channel must be optimized
10. Restore the old value for **wbsw**, **wbst** and the sample rotation
11. Terminate the **atma** command with a specific status (description in chapter: Command Status). If optimization was not successful, a window with a message will be shown.

4.1.3 atmm process

The command **atmm** allows the positions of the tuning and matching rods of the probe to be operated directly via the workstation.

atmm will do the following steps:

1. Check if one of the actuators is on the end stop and has to moved away.
2. Initializing the actuators if needed ([see “Actuator Initialisation” on page 6-5-30.](#)).
3. Read the probe information from the PIC system and get information of the routed channel in TOPSPIN (e.g. **edsp**)
4. Set the optimal wobble width (**wbsw**) and the number of wobble steps (**wbst**) for the chosen channel
5. Set the broad-band or switched channels, to the configured nucleus.
6. Start a special wobble process to get the best resolution. The wobble curve may look unfamiliar
7. Open a window showing the various controls to operate the matching and tuning rods (see next chapter: **atmm** graphical user interface)
8. Stop the wobble process and confirm storing the tuning and matching information.
9. Restart the process at step 4, if another channel was selected
10. Restore the old value for **wbsw** and **wbst**
11. Terminate the **atmm** command with a specific status (description in chapter: Command Status)

4.1.4 atmm control window

The command **atmm** will open the control below.

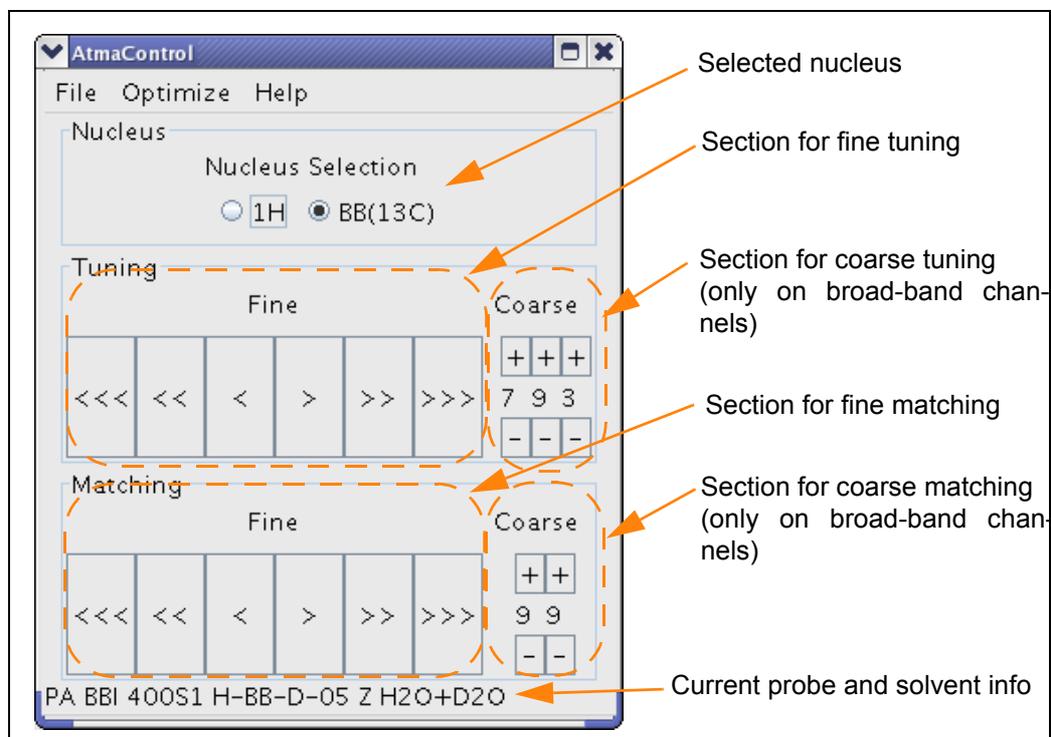


Figure 4.1: The atmm control window

4.1.4.1 Menu structure

- **File -> Save Position**
Save the current actuator positions, see also ["Stored Tuning and Matching Values" on page 31](#).
- **File -> Quit**
Close the window and terminate **atmm**. When changed, a dialogue asks if the new position should be stored.
- **Optimize -> Start**
Starting the atma process
- **Optimize -> Stop**
Stopping the atma process
- **Help -> Probe-Info**
Shows information about the probehead
- **Help -> Version**
Shows version of the ATMA server
- **Help -> Options**
Shows the available options for the ATMA commands atma and atmm

4.2 Options for *atma* and *atmm*

The table shows the available options for the commands *atma* and *atmm*.

Option	<i>atma</i>	<i>atmm</i>	Description
low	X	X	wobbles with all routed nuclei starting at the lowest frequency. This is also the default option
high	X	X	wobbles with all routed nuclei starting at the highest frequency
f1 - f8	X	X	wobbles the specified channels in the given order; example, f1 f3 f2 f1
xchannel	X	X	wobbles all routed X channels, example on TXI 13C & 15N
proton	X	X	wobbles the proton-channel
selectNuc	X	X	on broad-band probes, sets the broad-band channel to the configured nucleus and terminates the <i>atma</i> command. No optimization will be done
ext50	X	X	takes the reference with a external 50Ohm terminator, instead using the internal 50Ohm reference. If the wobble process takes a long time to optimize, the reference may drift away
version	X	X 1)	shows the actual ATMA software version. No optimization will be done
probeInfo (= bbInfo, drivePos)	X	X	shows information of the connected probe head, about broad-band and switched nuclei and the position of the drives. No optimization will be done
? (= options)	X	X	shows all available options for <i>atmm</i> and <i>atma</i> . No optimization will be done
manWbsw		X	use the actual wobble width (<i>wbsw</i>) and the number of wobble steps (<i>wbst</i>) for the wobble process
acqu	X	X	read SOLVENT information from current data set (eda, curdat/. .acqu) and not from global locksolv file
changePositionSet '#'	X	X	change the number of position set used for this nucleus by setting '#' [0, 1(default) ... 10]
stop	X		stop a running <i>atma</i> optimization ('atmopt' in the status line)
exact	X		gets the best optimization but can take a long time to complete
coarse	X		is faster to complete but will perform a less accurate optimization
noWin	X		shows no message window if <i>atma</i> couldn't find the optimum. Useful for scripts
storeWobb 'PROCNO'	X		store wobble data, data is stored with passed PROCNO

Table 4.1: *atmm* and *atma* options

1) Works only when a probehead with ATM Accessory is connected.

4.2.1 Examples for atma and atmm

- **atma** or **atma low**
will automatically tune and match all observable routed channel starting at the lowest frequency
- **atma f2 coarse**
atma f1 exact
optimize tuning and matching for f1 (e.g. 1H) very accurate and for f2 (e.g. 13C) fast
- **atma proton**
optimize tuning and matching only for 1H
- **atma xChannel**
optimize tuning and matching for all routed channels (13C, 15N), except for 1H
- **atma selectNuc**
sets the broad-band channel to the requested and terminates the **atma** command. No optimization will be done
- **atma f1 f3 f1 noWin**
will automatically tune and match the channel f1, f3 and again f1. If it get an error no message window will be shown
- **atmm f1 manWbsw**
starts the wobble process on channel f1 using the actual wobble width (**wbsw**) and the number of wobble steps (**wbst**)
- **atma version**
shows the version of the installed ATM software and the release notes

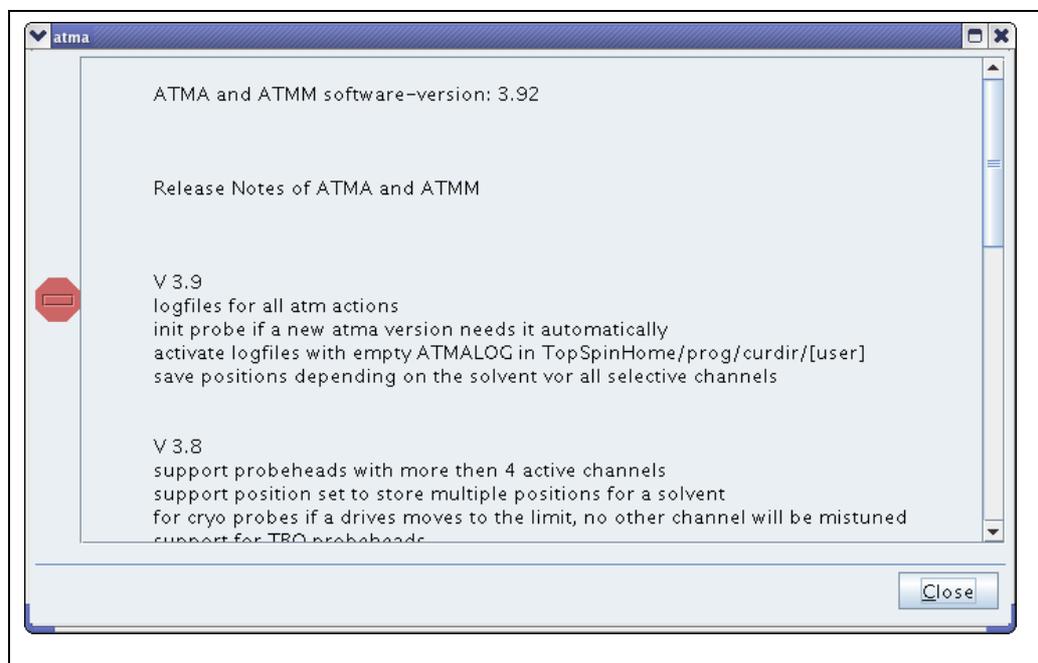


Figure 4.2: The atma version window

- **atma probeInfo**
shows the message window below

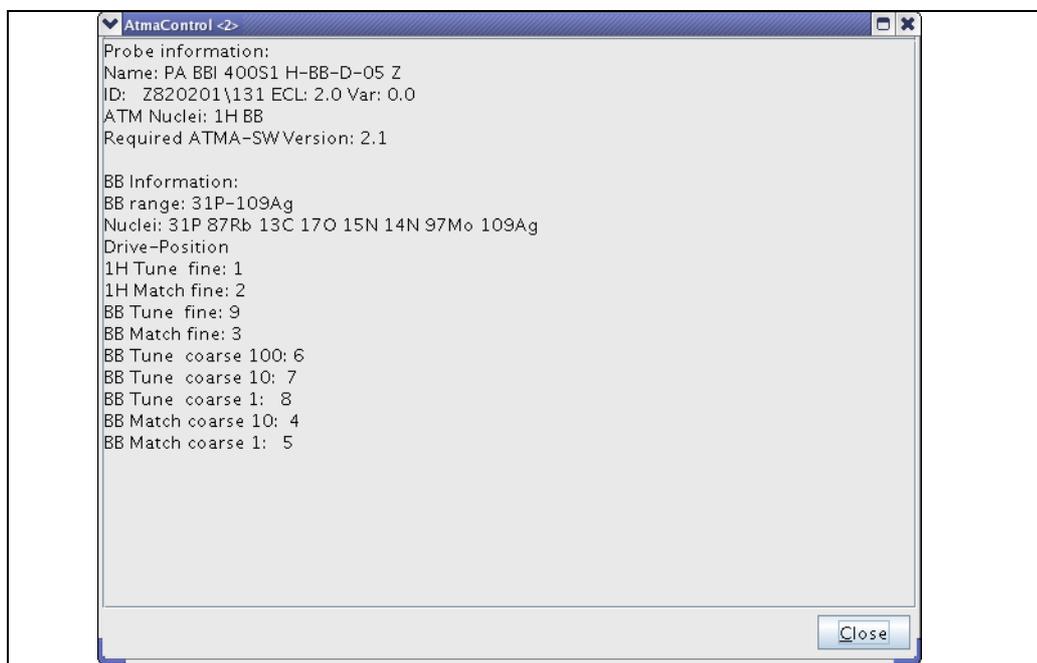


Figure 4.3: The probe info list

- **atma changePositionSet 5**
is setting up atma to work with 5 different settings where the optimum for the tuning and matching is expected.
- **atma f1 acqu**
is tuning and matching f1 with the solvent information read from the current dataset.
- **atma f1 storeWobb 10**
is optimize tuning and matching for f1 and stores the result to 'PROCNO' 10.

4.3 Verify a new nucleus on the broad-band channel

To set up the broad-band channel for a new nucleus the following steps must be done:

1. Check with the command **atmm probeInfo** if the nucleus can be used with the probe. The range of the broad-band channel is shown e.g. "31P-109Ag".
2. Connect the broad-band channel to a HPPR module which can wobble the requested nucleus, e.g. 2H or 19F can't be wobbled on some modules.
3. Configure the nucleus with the **edasp** command (start with a low frequency nucleus, because they are easier to set up).
4. Start the command **atmm** to verify the new nucleus. This must be done once for every new nucleus (Note: this is also true for the factory predefined nuclei which are shown in brackets in the bblInfo window)
The wobble width (**wbsw**) will be set very large. So the dip should be visible.
5. First use the tune coarse buttons (+ and -) to set the dip in the middle of the window, then use the match coarse button to get a good matching
If no dip is visible set the wobble width manually. Exit the **atmm** command (don't save the position) and set the wobble width with **wbsw**. Now restart the **atmm** command with **atmm manWbsw**.
6. Use the fine buttons (<, <<, <<<, >, >>, >>>) to get an optimized dip.
If the button colour is red, the dip can't move further in this direction. Set up the coarse position again (last step).
7. To check the position of the coarse buttons do one step up and down. The best position should now be between the two.
8. Close the **atmm** window and save the new position.
9. **atmm probeInfo** should now show the new nucleus.

4.4 Specialities

4.4.1 1H and 19F with QNP switch

If your probehead can observe 19F and decouple 1H (eg: QNP F-P-C-H), and you have only one 1H amplifier with a QNP switch (using the zgfhig pulse program to switch), then the ATMA fails to tune the 1H. It tries to tune both the 19F and the 1H using the X-BB preamp because the path for 1H to the 1H preamp is not in edasp.

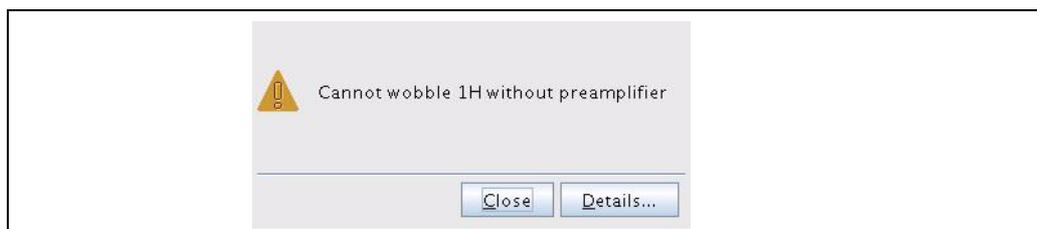


Figure 4.4: Atma fails to tune 1H

- i** Run *atma* for each channel separately with two different datasets using only one nucleus for each dataset. Start with the 19F channel first and do the 1H afterwards.

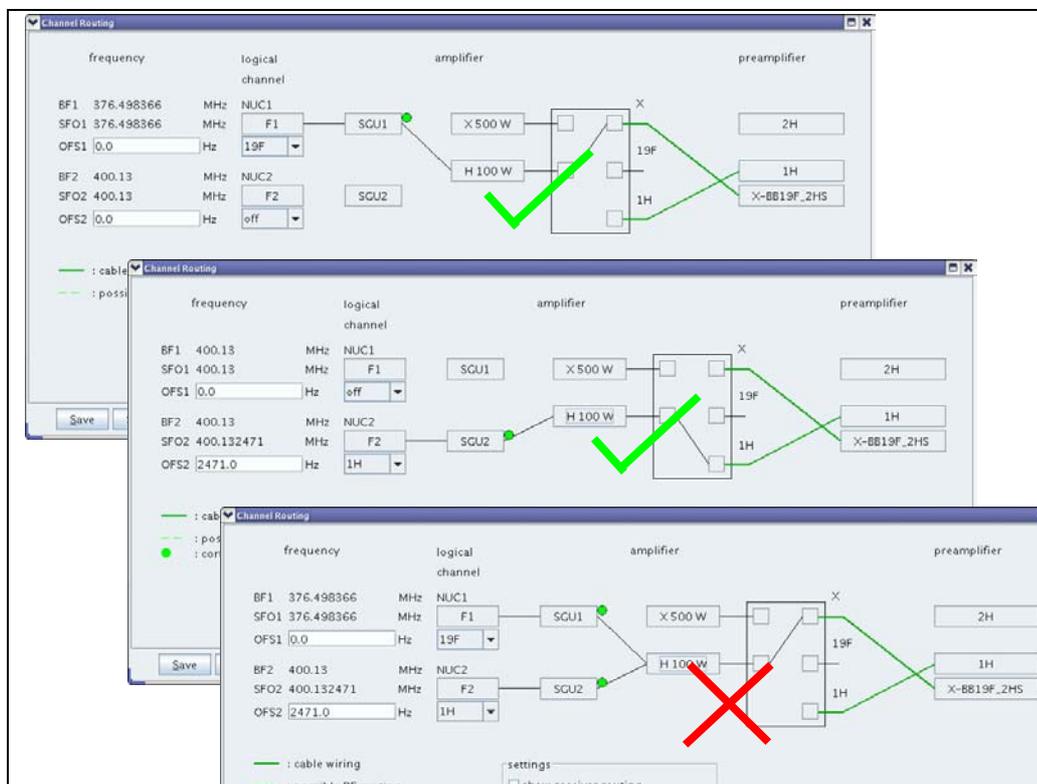


Figure 4.5: Routing 19F to 1H

4.4.2 Two 19F Channels

On some probe heads you can set the broadband and the proton channel to 19F. Those probeheads are labelled for example "BBF-H&F-D". In this case you have to take care to not mix up the two channels.

TopSpin sets the routing for the 19F regarding the sensitivity.

Probehead Type	Default channel for 19F
Observe	Broad band (BB)
Inverse	Proton and fluorine (H&F)

Table 4.2: Default channel for 19F

To force TopSpin not to use the default, you have to occupy the second possibility for 19F by routing an unused channel. Then run the *atma* command with the *f1* or *f2* option.

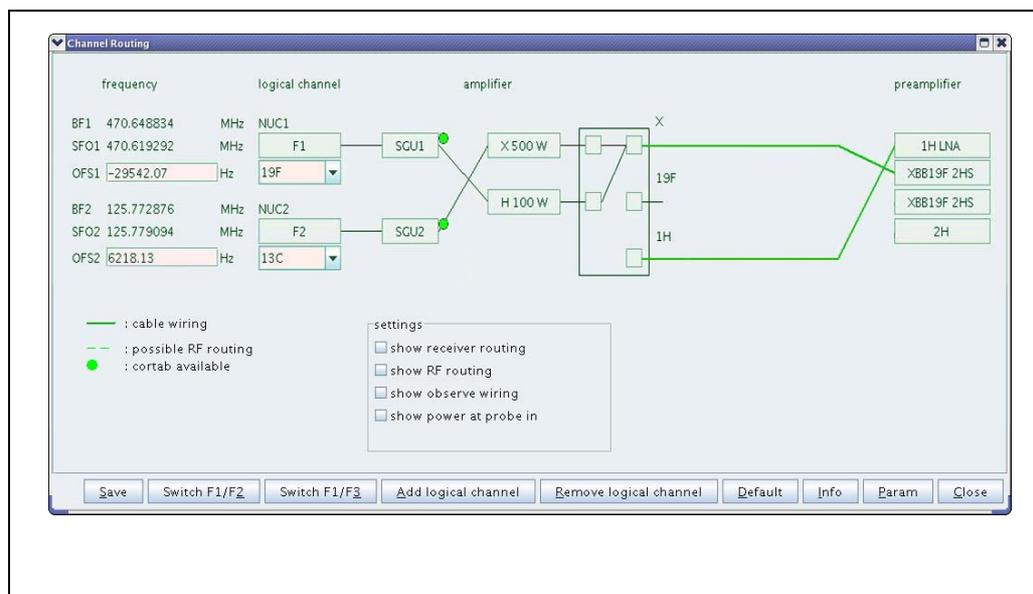


Figure 4.6: Routing 19F to 1H

4.4.3 Internal HPPR and no Position Detection

Since the internal HPPR 1H/2H module has a built-in 19F filter, the visible area of the wobble curve is very narrow. After a sample change on a inverse probe, the shift from the sample can be too high. ATMA may not see the dip any more and tries to find the dip blind. This may work but very often it does not.

This is way ATMA stores the positions according to the solvent. So it has good starting positions after a solvent change. In this case a position detection is required (see "Actuator Initialisation" on page 6-5-30.).

5 ATMA Knowledge

5.1 ATMA Software Architecture

The ATMA software was built as server and client. When using an **atma** or **atmm** command for the first time in TOPSPIN, the server will be started. From then the ATMA server is running, all the ATMA commands will run as a temporary active client.

The environment variables for the ATMA server will be set only once when the server is started. When having problem with the ATMA, close the whole TOPSPIN application, in order to stop the ATMA server.

5.2 Installing ATMA Patch

TOPSPIN and its patch levels comes with an ATMA server. But you can manually download and install an newer version of the ATMA server. This may be required if a new feature was included in a ATM server version but a new TOPSPIN patch level has not been released.

i The ATMA server is part of the TOPSPIN software and its patch levels.

i Make sure to use ftp binary mode when downloading files from ftp server. If you are using ftp ASCII mode the archive files will be corrupt.

To install a new ATM Patch do the following steps

1. Verify with the command **atmm version** if the installed ATM Version is older then the latest available version
2. Get the latest version from the Bruker ftp-server.
<ftp://ftp.bruker.ch/pub/NMR/download/atm/>
3. Copy the file or files to the correct folder. Do not forget to backup the old file version. See "ATMA Files and Folders" on page 6-5-35. for the correct folder.
4. Restart the TOPSPIN software.
5. Verify with the command **atmm version** if the installed version is running.

5.3 Actuator Initialisation

Some ATM Accessory will start with an initialisation procedure what is used to work with position detection. This depends on probe head age and type. To find out for what position detection is used, read "[Stored Tuning and Matching Values](#)" on page 31.

i Depending on the probe head the initialisation can take a some minutes.

Probe head	Position detection	Initialisation
QNP and QNI (RT probe and CRR), MNP (CRP)	Yes	Yes
RT broad band probe heads	Yes	Yes
RT inverse probe heads produced after 2007	Yes	Yes (from 3.921) 1H (before 3.92)
Other RT probe heads produced after 2007	Yes	Yes (from 3.92) No (before 3.92)
Other RT probe heads produced before 2007	No	No
Other cryo probes	No	No

Table 5.1: Actuator Initialisation

The following table indicates, in which case the initialisation is proceeded.

Initialisation trigger	RT probes	Cryo probes
Command atma or atmm after HPPR power failure	x	x
Command atma or atmm after PICS cable connected	x	x
Command atma or atmm after actuator unit attached to probe head		x

Table 5.2: Initialisation Trigger

5.4 Stored Tuning and Matching Values

ATMA is storing values into a file in order to provide a start value for finding the dip on subsequent NMR tubes. Read the following pages about what is stored and when the values are stored.

The files, in which the information is stored, has the extension ".bb". To locate the file in the file system see [See "ATMA Files and Folders" on page 6-5-35.](#)

The following file is an example file with the ".bb" extension. This file contains all the different specialities. The important part of the line is printed bold.

i The "@" character is used to mark different position sets in the ".bb" file. Do not confuse ATMA by using solvent names containing this character.

```

line 01  $probebbsets,1.0,31P,+799.0174,+99.0320,+110.00,+005.00,+000.40,+000.10#
line 02  $probebbsets,1.0,87Rb,+798.0182,+99.0275,+110.00,+005.00,+000.40,+000.10#
line 03  $probebbsets,1.0,13C,+795.0108,+99.0124,+180.00,+005.00,+000.40,+000.10#
line 04  $probebbsets,1.0,2H,+785.0365,+87.0226,+180.00,+005.00,+000.40,+000.10#
line 06  $probebbsets,1.0,17O,+777.0260,+92.0096,+180.00,+005.00,+000.40,+000.10#
line 07  $probebbsets,1.0,15N,+758.0104,+78.0231,+210.00,+005.00,+000.40,+000.10#
line 08  $probebbsets,1.0,14N,+709.0261,+65.0140,+210.00,+005.00,+000.40,+000.10#
line 09  $probebbsets,1.0,97Mo,+687.0195,+59.0213,+210.00,+005.00,+000.40,+000.10#
line 10  $probebbsets,1.0,109Ag,+536.0135,+14.0155,+210.00,+005.00,+000.40,+000.10#
line 11  $probebbsets,1.0,19F,+002.0137,+00.0165,+093.10,+000.00,+000.00,+000.00#
line 12  $probebbsets,1.0,31P,+001.0092,+00.0170,+040.10,+000.00,+000.00,+000.00#
line 13  $probebbsets,1.0,13C,+000.0187,+00.0198,+096.10,+000.00,+000.00,+000.00#
line 14  $atmaposset,1.0,1H,1H,1M NaCl H2O+D2O,-001,+000.0008,+00.0006,+040#
line 15  $atmaposset,1.0,1H,19F,1M NaCl H2O+D2O,-001,+000.0008,+00.0006,+040#
line 16  $atmaposset,1.0,1H,1H,CDCl3,-001,+000.0019,+00.0034,+040#
line 17  $atmaposset,1.0,1H,1H,C6D6,-001,+000.0022,+00.0037,+040#
line 18  $atmaposset,1.0,1H,1H,Acetone,-001,+000.0015,+00.0039,+040#
line 19  $atmaposset,1.0,1H,1H,DMSO,-001,+000.0012,+00.0037,+040#
line 20  $atmaposset,1.0,1H,1H,D2O_S1000,-001,+000.0046,+00.0015,+040#
line 21  $atmaposset,1.0,1H,1H,H2O+D2O,-001,+000.0011,+00.0040,+040#
line 22  $atmaposset,1.0,1H,1H,H2O+D2O@1,-001,+000.0011,+00.0040,+040#
line 23  $atmaposset,1.0,1H,1H,H2O+D2O@2,-001,+000.0011,+00.0040,+040#
line 24  $atmainfo,1.0,+001#

```

Figure 5.1: Example ATMA ".bb" File

ATMA Feature	Probe Type	Example File	Description
Broad band channel nucleus position	Broad band (BBO, BBI)	Line 1 to 10	chapter 5.4.1 on page 32
Switching channel nucleus position	Switching (QNP, QNI, MNP)	Line 11 to 13	chapter 5.4.2 on page 32
Tunable channel nucleus position	Probe labelled: "1H&19F/..."	Line 14 and 15	chapter 5.4.3 on page 32
Solvent depending tuning and Matching	All selective channels (Probeheads with position detection)	Line 16 to 20	chapter 5.4.4 on page 32
Solvent Variations	All selective channels (Probeheads with position detection)	Line 21 to 23	chapter 5.4.4.1 on page 33
Initialisation Version	All	Line 24	-

Table 5.3: ATMA Features

5.4.1 Broad Band Channel Nucleus Positions

On a broad band channel the tuning and matching information for all nuclei is stored. For some of the nuclei there has already been stored a preset value in the PICS. For these nuclei you can start the **atma** command without any preparation work. For other nuclei in the frequency range (e.g. from ¹³C to ¹⁰⁹Ag) you have to run the **atmm** command first to set and store the tuning and matching values. The **wbsw** parameter is calculated for new nuclei.

You can see such tuning and matching positions in example file [Figure 5.1 on page 31](#) from line 1 to 10.

5.4.2 Switching Channel Nucleus Positions

On switched channels the tuning and matching information for the nuclei are stored in the ".bb" file. All the available nuclei and their **wbsw** parameters are defined in the PICS and cannot be changed.

You can see such tuning and matching positions in example file [Figure 5.1 on page 31](#) from line 11 to 13.

5.4.3 Tunable Channel Nucleus Positions

Some probe heads are equipped with a proton channel that can be tuned to fluorine as well. These probe heads are labelled for example: "¹H&¹⁹F/...." and treated like a switching channel. The tuning and matching information is stored independent for ¹H and ¹⁹F.

You can see such tuning and matching positions in example file [Figure 5.1 on page 31](#) line 14 and 15.

5.4.4 Solvent Depending Nucleus Position

All selective channels with position detection (See "[Actuator Initialisation](#)" on page 6-5-30.) will automatically store tuning and matching information together with the current solvent you have locked on. This is especially helpful if your channel is sensitive to the employed NMR solvent.

You can see such tuning and matching positions in example file [Figure 5.1 on page 31](#) from line 16 to 20.

i Changing the solvent with the **solvent** command does not set the solvent used for **atma** in any case. Use the **atmm** command to see the solvent in the footer in the window and the **atmm acqu** command to use the solvent of the current data set.

5.4.4.1 Solvent Variations / Position Set

When using salty solvent with different salt concentrations, it might be necessary to try different tuning and matching settings. You can manually set the ATMA to up to 10 different position sets for starting tuning and matching on selective channels.

With the **changePositionSet [0...10]** option after the **atma** command you can set the required numbers of sets.

Setting the number of position sets:

1. First set the tuning and matching manually with the **atmm** command.
2. Then copy this value into the new sets with **atma changePositionSet** and the required number.
3. Confirm the setting on the dialogue shown in [Figure 5.2](#).

Deleting position sets:

1. Delete all the positions sets or just the additional ones by setting the positions set variable to 0 or 1.
2. Confirm the setting on the window shown in [Figure 5.2](#).

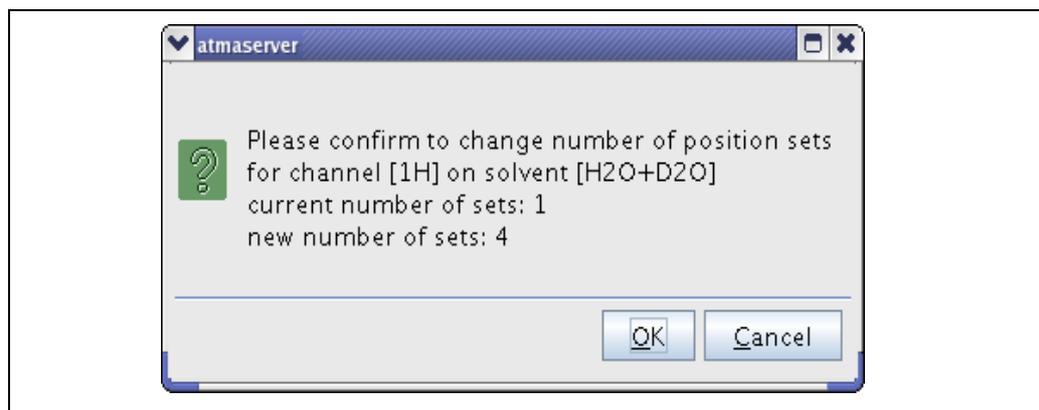


Figure 5.2: Changing Position Set

Such stored tuning and matching positions are given in the example file [Figure 5.1 on page 31](#) from line 20 to 23. In this example three position sets were used where line 20 corresponds to one position set and line 23 to 3 position sets.

5.5 Command Status

The *atma* and *atmm* commands return a status after termination. When writing user specific TOPSPIN macros, these status can be required. The status can take the following values:

Return value	Meaning
0	Command executed successfully
-1	Command not successful; resonance dip not found
-4	Aborted because a Stop Command was received
3	Communication failed (PICS)
6	System procedure error (wobble not possible)

Table 5.4: Status return values

5.6 ATMA Files and Folders

The following list shows files in a TOPSPIN installation used by ATMA.

These files are part of the installation and must not be deleted	
/opt/topspin/...	Description
conf/instr/servtool/hpprtool/tool/atma.hlp conf/instr/servtool/hpprtool/tool/atmamot.hlp	Atma help for HPPRtool
conf/instr/servtool/unitool/...	Atma help in UniTool
guide/man/acqref/atma.html guide/man/atma guide/man/atma/contents.htm guide/man/iconnmr/images/atma.PNG	ATMA description used by TOPSPIN help.
prog/docu/english/xwinproc/html/atma.html prog/docu/english/xwinproc/pdf/Atma.pdf	ATMA description
prog/mod/atmaclient prog/mod/atmaserver	ATMA server and client
conf/instr/[curinst]/probeheads/curprobe	Current probe head / ATMA in use

Table 5.5: ATMA Files and Folders from the Installation

These files are generated by ATMA and can be deleted	
/opt/topspin/...	Description
prog/curdir/[user]/ATMALOG	Control file for ATMA logging. Available from ATMA version 3.91. See “Starting ATMA Logfile” on page 6-5-39.
prog/curdir/[user]/AtmaServer.ref	CORBA reference to ATMA server.
prog/curdir/[user]/stderr.AtmaClient.log prog/curdir/[user]/stderr.AtmaServer.log prog/curdir/[user]/stdout.AtmaClient.log prog/curdir/[user]/stdout.AtmaServer.log	ATMA default logfiles.
conf/instr/[curinst]/probeheads/xxxx_xx.ph	Cached PICS files for fast access. Auto generated and updated by ATMA
conf/instr/[curinst]/probeheads/xxxx_xx.pha	Cached PICS files from CRP ATM actuator unit for fast access. Auto generated and updated by ATMA
conf/instr/[curinst]/probeheads/xxxx_xxxx_xx.par	PICS information used by edhead in jcamp format. Auto generated file by edhead.
conf/instr/[curinst]/probeheads/xxxx_xx.bb	Stored ATMA values.

Table 5.6: ATMA Files and Folders used for ATMA Software

5.7 Troubleshooting

5.7.1 *atmm* or *atma* Errors

If *atmm* or *atma* generate an error, check the following points:

- Is the cable on the probe and HPPR plugged in?
- Is the HF cable attached to the correct channel of the probe?
- Is the corresponding nucleus observable (HPPR module)?
- Can the selected channel be wobbled with the standard *wobb* command?
- Try to move the matching and tuning with the *atmm* command.
- If the dip couldn't be optimized with *atma*, try a second time.
- If the requested nucleus couldn't be set on broad band probes, remove the PICS System connector on the probe and then re-connect it.
- Restart the ATMA server by restarting TOPSPIN.
- Are the filters according to the filter manual?
- Does the RT probe has a position detection? (See ["Internal HPPR and no Position Detection" on page 5-4-27.](#))

5.7.2 Checking Communication with ATMA

If you can download the PICS file from the probe head or ATM actuator unit, the communication is working. Depending on the HPPR different tools are used.

HPPR type	HPPRtool	UniTool	Web interface
HPPR/1	x		
HPPR/2		x	
Internal HPPR		x	x
Read details in...	chapter 5.7.2.1 on page 37	chapter 5.7.2.2 on page 37	chapter 5.7.2.3 on page 38

Table 5.7: Communication with ATMA

5.7.2.1 Communicating with HPPRtool

1. Type "hppr" in a shell on a Linux system or on the command prompt on a Windows system.
2. After the start screen appeared, press "y" to continue
3. In the main menu Press "8" to select "Board function HPPR-Controller..."
4. Press "7" for the "PICS Function..."
5. Press "1" "Read Probehead PICS-Information"
6. This action will take some time. Wait until the PICS is shown in the window. If the PICS appears the communication between HPPR and ATMA is working.
7. Press "return" and "q", "q", "q", "y" to quite the program.

5.7.2.2 Communicating with UniTool

1. Type "UniTool" in a shell with a Linux system or on the command prompt on a Windows system.
2. Enter the device name "hppr"
3. Confirm the address 80 by pressing "return"
4. After the start screen appeared, press a button to continue
5. In the main menu Press "i" to select "CRP/ATMA/PICS ..."
6. For a RT probe press "P" to select "Show PICS"
For a CRP press "B" to select "Show CRP-ATMA BIS"
7. Wait until the PICS is shown in the window. If the PICS appears the communication between HPPR and ATMA is working.
8. Press "return" and "q", "x", "return" to quite the program.

5.7.2.3 Communicating through web interface

1. Type "ha" in the TOPSPIN command line.
2. Open the DRU web interface

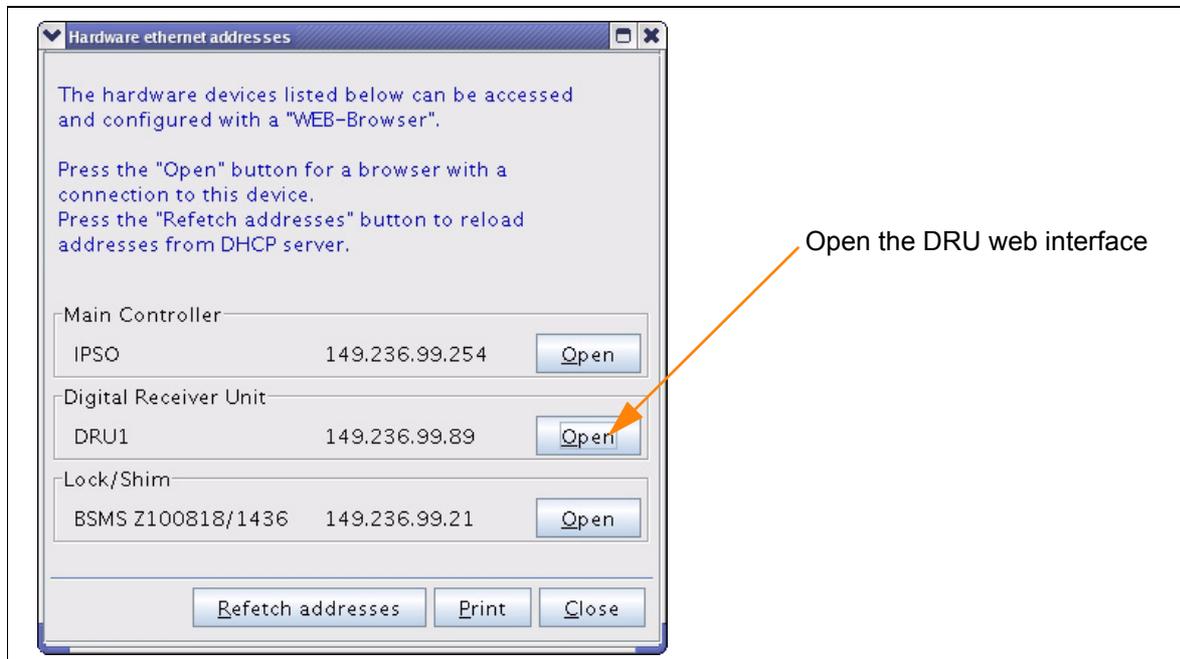


Figure 5.3: The DRU web interface

3. Select "AQS Hosted Devices" and then "HPPR/2 Overview"
4. For a RT probe press "read PICS" in the "CRP/ATMA/PICS" section
For a CRP press "read ATMA BIS" in the "CRP/ATMA/PICS" section

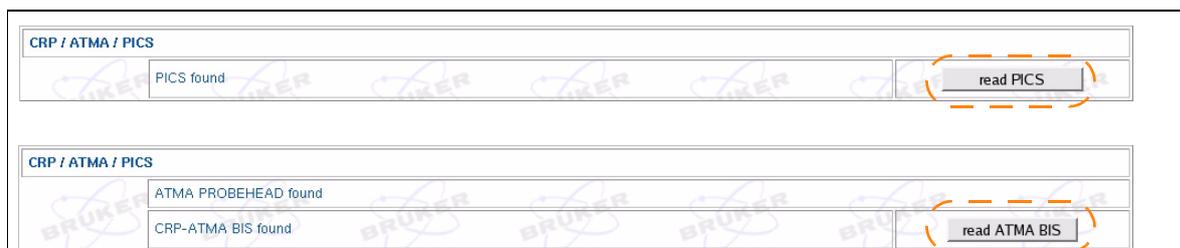


Figure 5.4: Reading PICS from DRU web interface

5. Wait until the PICS is shown in the window.
If the PICS appears the communication between HPPR and ATMA is working.
6. Close the browser window.

5.7.3 Starting ATMA Logfile

If a ATMA causes problems that can not be solved with the checklist under "atmm or atma Errors" on page 36 you should produce an atma logfile and send it, together with the *uxnmr.info* file and a problem description, to BRUKER for support.

There are two different ways to start the logging. Both ways give you the possibility of selection a path for the logfiles and a logging resolution level (0= nothing to 100=everything).

Logging modes	Persistency	Read details in ...
Command: debugmod	Will be stopped together with TOPSPIN.	chapter 5.7.3.1 on page 39
File: ATMALOG	Will last as long as the file exists.	chapter 5.7.3.2 on page 40

Table 5.8: Different logging Modes

5.7.3.1 Start logging with debugmod

- Restart TOPSPIN and do not use any ATMA commands.
- Type the command **debugmod** in TOPSPIN.
- Select a path for the ATM logfile.
- Set the debug level to 100.

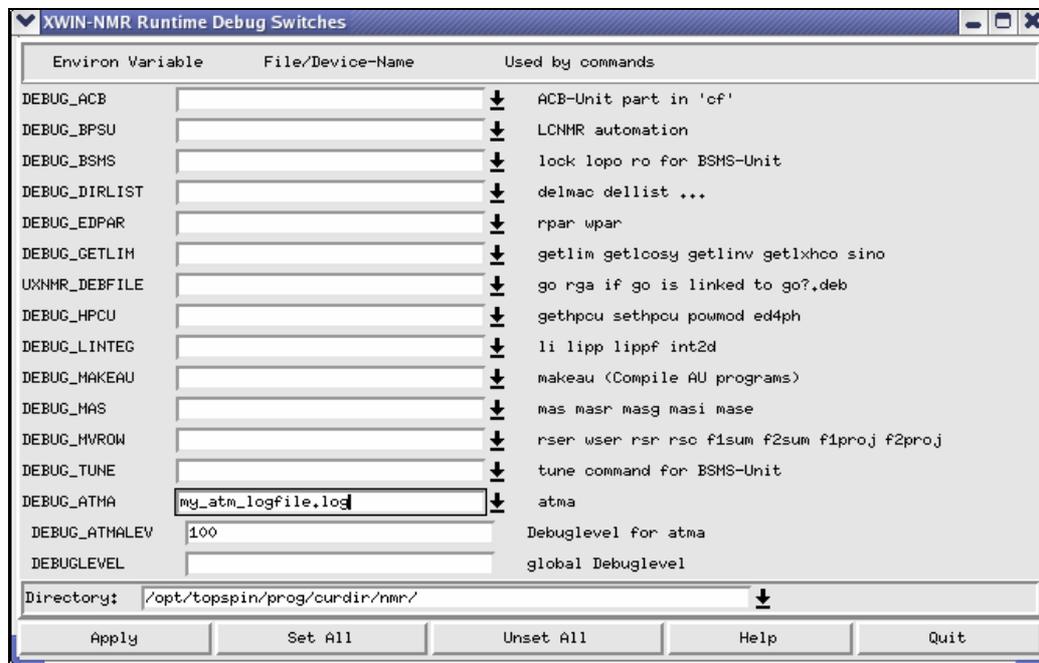


Figure 5.5: The debugmod window

5.7.3.2 Start logging with the ATMALOG

If the commands **atma** or **atmm** will find the text file ATMALOG in the file system on the path `/opt/topspin/prog/curdir/[user]/ATMALOG` the logging is enabled immediately.

File Content	Logfile path	Level
Empty text file	same as ATMALOG	100
Text file with: "[path] [level]"	from File	from File

Table 5.9: Different logging Modes

```
line 01 /home/nmr/myatmalogfiles/ 80
```

Figure 5.6: Example ATMALOG File

6 Contact

Submit your inquiries regarding ATMA to your local BRUKER BIOSPIN representative. Use the following address to acquire further information.

6.1 Manufacturer

Bruker BioSpin AG
Industriestrasse 26
CH-8117 Fällanden
Switzerland
Phone: +41-44-825-91-11
Fax: +41-44-825-96-96
<http://www.bruker.com>

Please refer to the Model No., Serial No. and Internal Order No. in all correspondence regarding the MR system or components thereof.

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A.4 Glossary

ATM Accessory

Automatic Tuning and Matching

BASH

Bruker Advanced Service Handbook

Broad-band channel

A range of nuclei on a probehead channel.

CRP

CRyo Probe

HPPR

High Power PReamplifier

Inverse

Probe with ^1H on the inner, most sensitive coil

Observe

Probe with ^1H on the outer, less sensitive coil

PICS

Probe Identification and Control System

RT

Room Temperature

S/N

Signal to Noise

Selective channel

One fixed nucleus on a probehead channel.

Switched channel

Several fixed nuclei on a probehead channel.

TOPSPIN

Bruker software for acquisition, processing and analysis

Tunable channel

A probe channel with an extended tuning range.

A.5 References

- [1] BRUKER Site Planning AVANCE Systems 300-700MHz (Z31276)
Stanley J. Niles / Daniel B. Baumann, February 24, 2008
Bruker Biospin GmbH, Rheinstetten, Germany
- [2] BRUKER Site Planning AVANCE Systems 750-950 MHz (Z31686)
Razvan Teodorescu, August 28, 2006
Bruker Biospin GmbH, Rheinstetten, Germany

A.6 Revision History

Index	Date	Who	Alteration Type
001	18.6.1999	SSV	First release
002	21.2.2000	SSV	Broad band probe heads added
003	2.4.2009	SRE	From XwinNMR to Topspin HPPR/2 added CRP ATM added

Table A.1: The Revisions of this Manual

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